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Structure of stacked InAs quantum dots in a Si matrix: HRTEM experimental results and modeling

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Abstract. A quantum dot structure containing two layers of small coherent InAs clusters embedded into Si single crystal matrix was grown by MBE. The structure of these clusters was investigated by high resolution transmission electron microscopy. The quality of the grown structure severely depends on the substrate temperature, growth sequence, and the geometrical parameters of the sample. Investigation demonstrate that Si crystal can incorporate only a limited volume of the deposited InAs in a form of coherent clusters.

Introduction

There is a strong interest in combining unique properties and flexibility of III–V materials with silicon technology, which is ideally suited for microelectronics. Until now most of researchers are concentrated on growth of thick layers of III–V materials on silicon [1]. More recently, the idea of using of ultra-small coherent III–V narrow gap crystallites (quantum dots) coherently inserted in the silicon matrix has been proposed [2]. Scanning tunnelling microscopy studies demonstrates that small InAs quantum dots (QDs) can be, indeed, formed on the Si(100) surface, and, after overgrowth with Si, these QDs demonstrate intense and broad luminescence line at about 1.3 μm at 10 K [3]. Despite of the high importance of these spectroscopic results no direct proof of the coherent nature of the InAs insertions in a silicon matrix was given.

The aim of this paper is to demonstrate the possibility to characterise InAs insertions in a Si matrix using high resolution transmission electron microscopy (HRTEM), to prove the coherent nature of InAs inclusions, to compare experimentally derived and simulated HRTEM images to draw conclusions on the QD size, and to demonstrate the possibility of growth of coherent multiple InAs insertions in a Si matrix for applications in micro- and optoelectronics.

Experimental

The samples were grown using a molecular beam epitaxy (MBE) on Si (100) substrates. The variable parameters were the substrate temperature during growth, the InAs growth rate, the average thickness of the insertion and the arsenic pressure during growth. Two samples (A and B) were mostly investigated in this work (Fig. 1). The crystalline quality of the structure and the composition of the grown layers were investigated by HRTEM and the energy-dispersive X-ray spectroscopy (EDX). Computer simulations of HRTEM images were performed by using MacTempas program package [4].

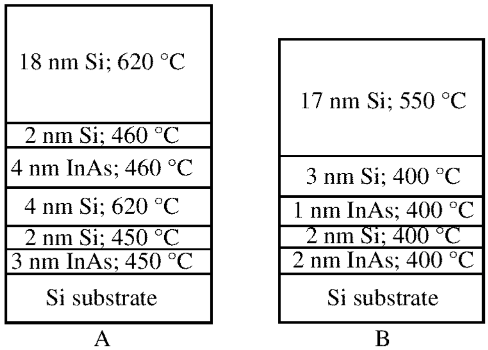

Fig. 1. Sequence and thickness of the layers in two MBE grown structures: A and B.

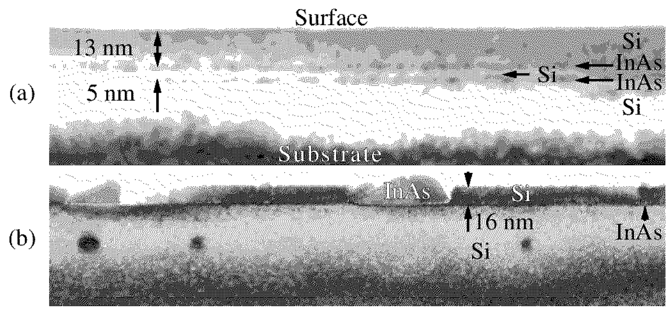

Fig. 2. Cross section TEM images of the specimen A (a) and B (b). Two layers of InAs clusters are marked by arrows in (a).

Results

A cross section TEM image of sample A taken at low magnification is shown in Fig. 2(a). Two InAs insertions exhibiting dark contrast are marked by arrows. One can also notice that the effective thickness of the InAs insertions is well below 4 nm, indicating that only a small part of the deposited InAs was incorporated into the structure after Si overgrowth. The reason for this is the increase of the substrate temperature after the InAs deposition and overgrowth of ultra-thin (2 nm) Si layer. We found this step to be important to keep the high quality of the structure, because part of the excess of deposited InAs is effectively evaporated at 620 °C. In the case of the sample B, where the InAs and Si deposition occurred at lower temperature (Fig. 2), the most of InAs is concentrated in large dislocated clusters. In this case it is clearly seen that the Si overgrowth does not take place in the vicinity of the InAs clusters. Moreover, only the lower InAs layer shows a coherently incorporated InAs clusters. At the surface specimen contains a high density of shallow pits (16 nm deep) partly occupied by large InAs precipitates. Plan-view TEM images of these precipitates demonstrate a square-type Moir^ pattern with a spacing corresponding to the misfit between Si and InAs. EDX spectra taken from these precipitates in the transmission mode demonstrate pronounced In and As peaks. To analyse the lattice structure and size of the InAs clusters incorporated in the Si matrix in sample A, cross-section samples have been investigated by HRTEM (Fig. 3). Contrast features having a size of about 3 nm in diameter and laterally separated from each other by 0.5-1 nm can be clearly seen (see arrows in Fig. 3). To understand the origin of these contrast features computer simulations

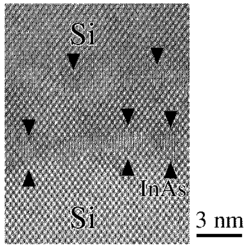

Fig. 3. Cross section image of the sample A taken at high resolution. InAs clusters are marked by arrows.

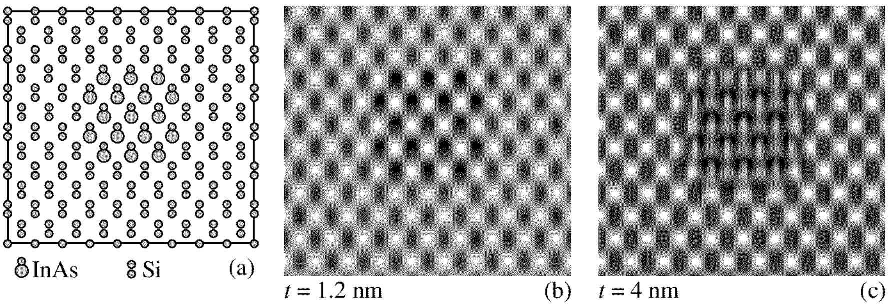

Fig. 4. Atomic model of the InAs cluster in a Si matrix (a) and two high resolution images simulated for crystallite size of 1.2 (b) and 4 nm (c).

of the small InAs cluster in Si matrix have been done. The crystallographic model of the InAs cluster used for the calculations is shown in Fig. 4(a). The model represents the case, when Si atoms are substituted with InAs molecules, reducing the symmetry of the matrix. The HREM simulations are carried out for imaging conditions close to the experimental ones (Scherzer defocus) and for different foil thickness (Fig. 4(b,c)). For the small thickness ($t = 1.2$ nm) the contrast is fairly low, as it may be expected, while in the case of thicker crystal ($t = 4$ nm) the theoretical image demonstrates rather good agreement with experimental one (Fig. 3).

Discussion

To summarise the results one can conclude that layers of coherent InAs insertions can be successfully fabricated in a single-crystalline silicon matrix. Quality of the grown structure severely depends on the substrate temperature, growth sequence, and geometrical parameters of the sample. In addition to STM results, one can also conclude that the Si crystal lattice can only adopt a limited volume of the deposited InAs in a form of coherent clusters. If the deposited InAs layer is too thick, large dislocated InAs precipitates are formed accumulating excess of InAs during Si overgrowth. We also note that the total area occupied by the shallow pits (see Fig. 2(b)) was about 2 times lower in sample A than in B. Besides, these pits in sample A are almost empty, while in the sample B they always contain relaxed InAs clusters. Thus, high temperature step in Si overgrowth is essential to evaporate the excess amount of InAs.

From the above considerations, and taking into account the STM data [ ] it appears that the average thickness of deposited InAs, the thickness of the Si spacer between the InAs insertions, the substrate temperature during the InAs deposition and Si overgrowth should

be optimised to obtain high quality structures with multiple InAs insertions in Si.

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